Hybrid Parallel Finite Difference Time Domain Simulation of Nanoscale Optical Phenomena

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Abstract

The increasing computational demands of finite-difference time-domain simulations for studying optical phenomenon requires codes with very high performance. This paper introduces a new hybrid parallel code using standard MPI and OpenMP technologies. The code is portable to a variety of high performance systems. The transmission of light through an isolated sub-wavelength in an optically thick silver film is outlined as an example application of the code.

1 Introduction

The report of enhanced optical transmission through an array of nano-scale holes by Ebbesen et al. [1] in 1998 has led to a lot of interest in the phenomenon and its applications. Enhanced transmission is observed when the surface of a thin film of metal is patterned with some arrangement of periodic features, such as an array of perforations, where each hole is much smaller than the wavelength of the incident light. Surface plasmons have been generally accepted as the waves determining the behavior of the periodic structures at optical frequencies and much has been learned about their propagation and possible applications in photonic technologies. Experiments and theoretical analyses have helped to understand the nature of the enhanced light transmission, and to provide some quantitative approaches to predicting resonant wavelengths for some, but not all, geometries. It has been pointed out by Garcia-Vidal, et al. [2], and is apparent from the analyses published so far, that "calculations of transmittance spectra for a finite structure..., using a realistic dielectric function, are a computational tour de force that are beyond reach at the moment...". Design and optimization of devices that are relevant in practical applications of nano-structures cannot be achieved by approximate analyses. It is particularly difficult to include thin layers (on the order of $\lambda/4$) of dielectrics on one or both faces of the film, rectangular or elliptical holes, holes in combination with circular corrugations, asymmetric arrays, and similar structures that are of practical importance.

The finite difference time domain (FDTD) is the best suited method for solution of these problems, and its use has been previously reported [3]. However, for many structures of practical interest, single platform codes do not provide sufficient computational resources. In this contribution, we describe a new hybrid parallel code using standard MPI and OpenMP technologies. An example of the application is also given.

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE	2. REPORT TYPE	3. DATES COVERED
01 JAN 2005	**N/A**	**-**

4. TITLE AND SUBTITLE	5a. CONTRACT NUMBER
Hybrid Parallel Finite Dierence Time Domain Simulation of Nanoscale Optical Phenomena	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **Electrical and Computer Engineering University of Victoria Victoria, British Columbia, Canada**	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release, distribution unlimited

13. SUPPLEMENTARY NOTES
See also ADM001846, Applied Computational Electromagnetics Society 2005 Journal, Newsletter, and Conference.

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			
unclassified	**unclassified**	**unclassified**	**UU**	**4**	

2 Parallel FDTD Algorithm

2.1 Previous Implementations

Since its introduction to electromagnetics by Yee, FDTD has become very popular and highly developed [4]. Numerous parallel codes have implemented FDTD [5]. Most older parallel codes have been targeted at specialized vector supercomputers, which are very expensive compared to the clustering approach [6] that has now become common. Clusters of commodity computers, or nodes, rely on a high speed network to connect them together. A message passing system allows the nodes in the cluster to exchange information as needed during the execution of an algorithm. The most common message passing system is Message Passing Interface (MPI). A less common, older system is Parallel Virtual Machine (PVM).

The FDTD algorithm is well suited to implementation on a cluster. Updating a component of the electric or magnetic field depends only on the previous value of the field component in a given cell and on the field components in adjacent cells. The FDTD domain can be decomposed into a number of sub-domains, each of which can be assigned to a single node. Only the field components at the boundary between two sub-domains need to be passed between nodes, once per time step. This allows a FDTD code using MPI to increase its performance by processing multiple parts of the domain in parallel. It also allows much larger problems to be simulated, since the domain is divided into smaller parts which can individually fit into available memory, where the domain as a whole may be too large for a single machine.

A parallel implementation of the FDTD algorithm using MPI was described by Guiddaut and Mahdjoubi [7]. Since then, a number of other codes using MPI have appeared. Su et al. described an implementation of a FDTD using a OpenMP-MPI parallel hybrid [8]. OpenMP is an standard for shared memory parallelism which makes it straight forward to write code which can take advantage of symmetrical multiprocessors (SMP). Since OpenMP is supported by a number of major vendors, it is possible to write portable C/C++ or FORTRAN code which can be used on a number of different systems or compilers with little or no change. Using OpenMP and MPI together allow for significant flexibility, in that the code can be run on a cluster which has a number of single or multiple processor nodes, and on large shared memory systems such as the SGI Origin line.

2.2 Current Implementation

The application of FDTD to optics requires that the following algorithms be implemented:

- Perfectly Matched Layer (PML) absorbing boundaries to terminate the mesh.
- Wide-band plane wave excitation source, and a spatial two-dimensional Gaussian excitation.
- Lossy dielectrics described by dielectric constant and static conductivity.
- Drude plasma to characterize metals in the optical regime [9].
- Discrete Fourier Transform to extract frequency domain data from the time variation of fields.
- Scattering parameters extraction.
- Near-to-far-field transformation to obtain the transmittance and radiation patterns.

The OpenMP-MPI hybrid parallel FDTD algorithm is implemented as follows:

1. Divide FDTD problem domain into N sub-domains, where N is the number of nodes available to MPI. Since each node has its own memory, each sub-domain may be thought of as ranging from $(0, 0, 0)$ to (X, Y, Z).
2. Divide each of the N sub-domains into M chunks, where M is the number of processors available in each node.
3. Perform time stepping updates of the electric field components on each of the N nodes:

```
for i = (m-1)*X/M to m*X/M
  for j = 0 to Y
    for k = 0 to Z
      ex(i,j,k) = ex(i,j,k) + ...
      ey(i,j,k) = ey(i,j,k) + ...
      ez(i,j,k) = ez(i,j,k) + ...
    end
  end
end
```

   The value of m ranges from 1 to M. The first line of this pseudo-code shows how the update loops can be divided up among M processors using OpenMP. The complexity shown on the first line is handled by OpenMP.
4. Apply electric field boundary conditions and excitations. Data exchange between nodes using MPI is treated as a boundary condition and is handled in this step.
5. Perform time stepping updates of the magnetic field components on each of the N nodes.
6. Apply magnetic field boundary conditions and excitations, including MPI data exchange between nodes.
7. Repeat from 3.

3 Results

Degiron et al. have reported experimental evidence of surface plasmon enhanced transmission through a single isolated aperture in a thin silver film [10]. This problem is a good test case for the code because it is relatively small and can be evaluated quickly. Furthermore, it exercises critical parts of the code such as the Drude plasma model. Also, published experimental results are available for comparison with the simulations. The simulation set up consists of a 200x200x200 computational domain where the Yee cells are 5 nm along each dimension. The region is terminated by PML, and is excited by a Gauss modulated sine wave centered at 500 THz. Simulations were run for a square hole in a 300 nm thick silver film, where one dimension of the hole was fixed at 270 nm and the other dimension was different for each simulation. Each simulation was run for 3708 time steps, with a time step of 8.66e-18 seconds.

The execution times for various numbers of CPUs and nodes on an IBM RS/6000 SP with 8 nodes, each containing 16 375-MHz CPUs, are summarized in table 1.

# CPUs per node	# nodes	Runtime (seconds)
1	1	15180
16	1	4500
16	2	821

Table 1: Simulation execution times

4 Conclusion

A new parallel hybrid FDTD code using MPI and OpenMP technologies has been introduced. This code is significantly faster when run on a parallel computer than when only one CPU is available. The use of MPI allows for the simulation of very large problems by distributing the problem across multiple machines in addition to speeding the execution of the simulation by using more CPUs. The use of OpenMP makes it possible to utilize multiple CPUs, which share a single system image through shared memory. Together, these technologies enable the simulation of very large problems such as those involving thin layers of dielectrics, rectangular or elliptical holes, asymmetric arrays and other structures of practical importance is possible.

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